

This folder contains files that will come in hand for running multiple runs of HOLE on a ion channel protein. The steps to be followed are as follows:

Step 1: Open *hole.inp* and replace *pdbfilename.pdb* with the name of your pdb file.

```
7 ! note that HOLE input
8 coord pdbfilename.pdb
9 radius ~/hole2/rad/simp
10      ! n.b. can use
```

Step 2 (optional): You can modify the radius values the program uses to run the calculations by modifying the selection called *simple.rad*.

```
8 coord pdbfilename.pdb      ! Co-ordinates in pdb format
9 radius ~/hole2/rad/simple.rad ! Use simple AMBER vdw radii
10      ! n.b. can use ~ in hole
11
```

Step 3: Save the file *hole.inp*. Open terminal and run the command:

```
pgupta@mems13:../AutomationScripts/HoleAutomation$
expect script_100ROUNDS.exp
```

Step 4: The terminal will start running the HOLE calculations. Leave it undisturbed for ~10mins.

Step 5: Once the calculations have completed, open the file *holeshow2.tcl*.

Step 6: Replace the prot.pdb name with your pdb file's name. Save the file and close it.

```
1 proc loadh {j} {  
2 set k [expr $j+100]  
3 for {set i $j} {$i<$k} {incr i} {  
4 mol new prot.pdb  
5 mol delrep 0 top
```

Step 7: Open terminal and launch VMD. Once vmd has loaded, enter “source holeshow2.tcl” in the terminal window and press enter.

Step 8: Next, type “loadh 10” to load 10 runs of the HOLE calculations. Replace the number 10 with a number of your choice as desired.

